Phenol

108-95-2 | DTXSID5021124

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 195 °C

Global applicability domain: Inside

Local applicability domain index: 6.36e-01

Confidence level: 8.34e-01

Nearest Neighbors from the Training Set

Image not found
Phenol
Measured: 182
Predicted: 195

Image not found
Benzyl alcohol
Measured: 205
Predicted: 197

Image not found
m-Cresol
Measured: 202
Predicted: 197

Image not found
p-Cresol
Measured: 202
Predicted: 201

Image not found
o-Cresol
Measured: 191
Predicted: 201